IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant:	Harold E. Helson	Art Unit:	2128
Application No.:	09/502,133	Examiner:	Jones, Hugh M.
Filed:	February 11, 2000	Conf. No.	4787
Title:	Enhancing Structure Diagram Generation		

Commissioner for Patents
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AMENDMENT AND RESPONSE

This communication is responsive to the Office Action mailed on January 25, 2008, to which a response is due July 25, 2008 with a three-month extension of time. Accordingly, this response is timely filed.

Please amend the above-identified application as follows:

Amendments to the Claims are reflected in the listing of claims which begin on page 2 of this paper.

Remarks begin on page 6 of this paper.

Amendments to the Claims

This listing of claims will replace all prior versions, and listing of claims, in the application:

1. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

laying out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

outputting a representation of the chemical structure.

2-5. (canceled)

6-8. (canceled)

9. (currently amended) ~~Computer software, residing on a~~ A computer-readable storage medium encoded with~~, comprising~~ a set of instructions for use in a computer system to ~~help~~ cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes symmetrically equivalent atoms and bonds; and

lay out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

output a representation of the chemical structure.

10-12. (canceled)

13. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on rotational symmetry.

14. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on reflective symmetry.

15. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on inversive symmetry.

16. (previously presented) The method of claim 1, further comprising:

basing the identification on stereochemistry.

17. (previously presented) The method of claim 1, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

18. (previously presented) The method of claim 1, further comprising:

basing the identification on double bond stereochemistry.

19. (previously presented) The method of claim 1, further comprising:

determining a pivot point for the list.

20. (previously presented) The method of claim 1, further comprising:

determining a graph-theoretic center for the list.

21. (previously presented) The method of claim 1, further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. (previously presented) The method of claim 1, further comprising:

determining whether an atom belongs to the identified instance of chemical structural symmetry.

23. (previously presented) The method of claim 1, further comprising:

determining whether a bond belongs to the identified instance of chemical structural symmetry.

24. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is reflective, selecting a position on an opposite side of a mirror line.

25. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is rotative, selecting a position based on a pivot point.

26. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.

28. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

laying out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

outputting a representation of the chemical structure.

29. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on rotational symmetry.

30. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on reflective symmetry.

31. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on inversive symmetry.

32. (previously presented) The method of claim 28, further comprising:

basing the identification on stereochemistry.

33. (previously presented) The method of claim 28, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

34. (previously presented) The method of claim 28, further comprising:

basing the identification on double bond stereochemistry.

35. (currently amended) A ~~system~~ computer-readable storage medium encoded with a set of instructions to cause a system ~~for use in deriving~~ to derive a chemical structure diagram, the instructions causing the system to ~~comprising~~:

~~an identifier~~ identify~~ing~~ an instance of chemical structural symmetry in the chemical structure, wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

~~a positioner~~ lay~~ing~~ out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

~~an output device~~ output~~ting~~ a representation of the chemical structure.

REMARKS

Claims 1, 9, 28, and 35 are amended to clarify that which was already implicit in the claims and claim 5 has been canceled As a result, claims 1, 9, and 13-35 are pending, the remaining claims having been withdrawn from consideration. Support for the amendment is found throughout the specification, in particular at page 7-9 and in Figs. 4-5.

Interview

Applicant's representative, Mary J. Edwards, and the inventor, Dr. Harold Helson thank Examiner Jones and Supervisor Examiner Shah for speaking with them on July 22, 2008 regarding the claims and the pending Office Action. During the Interview, proposed claim amendments were discussed. The claim amendments presented in this response reflect the amendments discussed during the interview.

Rejection of Claims Under 35 U.S.C. § 102(b)

Claims 1, 5, 9, and 13-35 are rejected under 35 U.S.C. § 102(b) as being anticipated by Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis," Purdue University 1993 ("Helson thesis"). In particular, the Office Action refers to Algorithm 3.1 of the Helson thesis and suggests that repositioning allegedly uses symmetry information as recited in the pending claims. Applicant respectfully disagrees.

The Helson thesis does not teach or suggest (i) identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure; wherein the instance of symmetry includes symmetrically equivalent atoms and bonds; (ii) laying out symmetrically equivalent atoms and bonds in the chemical structure diagram to express the

identified symmetry; and (iii) outputting a representation of the chemical structure, as required by claim 1. Accordingly, the Helson thesis does not teach or suggest each claim limitation as required by § 102(b). Therefore, the Helson thesis does not anticipate claim 1.

To the extent the Helson thesis is concerned with symmetry at all, it is with respect to the perception of symmetry only. The Helson thesis does not disclose using symmetry information for laying out the atoms and bonds of a chemical structure diagram. Symmetry is discussed in the Helson thesis in chapter 4, with regard to the an aesthetic function, the AeF-Redraw algorithm, which "assesses how well a molecule or collection of molecules has been drawn." (Helson thesis, page 201). Symmetry is one of a number of criteria used by the AeF algorithm to assess the aesthetics of a chemical structure diagram. The Helson thesis discloses, "[t]he AEF that measures how well a given molecule of collection of molecules is drawn, AeF_Redraw, is composed of ten independent criteria, mixed together with different weightings…" (Id., page 203). Chapter 4 of the Helson thesis discloses that AeF_Redraw merely provides a numerical score for the relative aesthetics of the generated chemical structure diagram. Thus, symmetry is only discussed with regard to the AeF algorithm and the AeF algorithm is concerned solely with the perception of symmetry. The AeF algorithm does not teach or disclose laying out equivalent atoms and bonds to express a previously identified symmetry, as required by claim 1.

The Office Action refers to Algorithm 3.1, summarized at page 149 of the Helson thesis. Algorithm 3.1, the Redraw Algorithm, is discussed in detail at pages 148-156 of the Helson thesis. The Redraw Algorithm, however, does not use symmetry or the perception of symmetry for structure diagram generation. Significantly, nowhere in the description of the Redraw Algorithm is symmetry discussed, let alone laying out atoms and bonds to express a perceived symmetry. The Office Action also refers to the treatment of stereochemistry in the Redraw

Algorithm. The treatment of stereochemistry in the Redraw Algorithm is distinct from taking account of symmetry in laying out equivalent atoms and bonds in a chemical structure diagram. While the Redraw Algorithm takes account of stereochemistry to create an accurate chemical structure diagram, it does not attempt to identify equivalent atoms and bonds and lay them out to express a previously identified symmetry. Rather, the Redraw Algorithm provides for the projection angle of *trans* double bond substituents and the choice of wedge or hash marks for the bonds at a tetrahedral center. Accordingly, the Redraw algorithm of the Helson thesis does not teach or suggest each element of claim 1.

The Office Action further refers to repositioning with regard to the CAMEO program discussed in the Helson thesis. The respositioning algorithm discussed in the Helson thesis does not involve any assessment of symmetry, let alone laying out atoms and bonds in accordance with a perceived symmetry. Rather, "repositioning" refers to "positioning of the resulting molecules" in a chemical structure diagram relative to one another. (Helson thesis, page 145; see also id., page 173 ("As previously stated, repositioning is a separate problem and is executed by an independent package of routines. The subject of how to place molecules so that they are evenly distributed about the screen does not appear to have been broached in the chemical literature.")). "Repositioning" as the term is used in the Helson thesis, does not contemplate symmetry at all. Rather, "repositioning" assures that molecules are not crowded together on the display medium and that the empty space around the molecules is distributed relatively equally. Id. ("A good repositioning algorithm should: be fast; keep molecules large; put as much space as possible between molecules, and between molecules and screen borders; [and] distribute empty space equally, so that the void separating adjacent molecules is consistent."). It accomplishes these goals by drawing rectangles around the structures – without respect to any particular

feature of the chemical structure except its size – and arranging the rectangles so they are well distributed. (Id., pages 175-194, Algorithm 3.5 (page 177).). Accordingly, this part of the Helson thesis does not teach or disclose positioning or laying out atoms and bonds to express an identified symmetry, as required by claim 1.

For the foregoing reasons, the Helson thesis does not teach or suggest each and every element of the claims. Accordingly, the Helson thesis does not anticipate the claim 1. Claims 9, 28, and 35 have comparable limitations to those of claim 1. Accordingly, these claims, as well as the claims that depend from them, are not anticipated.

Rejection of Claims Under 35 U.S.C. § 103

In a previous Office Action, the claims were rejected under 35 U.S.C. § 103(a) as being unpatentable over Hu, et al., *Chemometrics and Intelligent Laboratory Systems*, 1/18/1999 (abstract) ("Hu"), or Shelley, et al., *J. Chem. Info. Comput. Sci.*, p. 247 (1979) ("Shelley"), or Fan et al., *J. Chem. Info. Comput. Sci.*, pp. 654-59 (1996) ("Fan") in view of the Helson thesis. The pending Office Action states that these rejections were withdrawn "in order to reduce the number of issues." (Office Action, page 13). Nevertheless, to advance prosecution, these rejections are addressed here.

As explained above, the Helson thesis does not teach or suggest laying out of atoms and bonds in accordance with a perceived symmetry. Therefore, the cited references, taken in combination, fail to teach or suggest each element of claim 1. (M.P.E.P. § 2143.03 (to establish a prima facie case of obviousness, all claim limitations must be taught or suggested by the prior art)). The secondary references do not cure the deficiencies of Helson.

The Office Action dated August 8, 2007 found that none of Hu, Shelly, or Fan disclose positioning atoms and bonds in a chemical structure diagram. (Office Action, page 9). The Office Action states:

> 9. Hu et al. disclose computer perception of topological symmetry from a connection table (see abstract).

> 10. Shelley et al. also disclose computer perception of topological symmetry from a connection table (see pg. 247).
>
> 11. Fan et al. disclose detection of constitutionally equivalent atoms from a connection table (see page 654).
>
> 12. Hu et al. or Shelley et al. or Fan et al. do not expressly disclose positioning the atoms and bonds.

(Id.). Moreover, in the Response dated October 29, 2007, Applicant explained, "Hu is concerned with the detection of topological symmetry, in a chemical structure, not the expression of such symmetry in a chemical structural diagram. Shelley, like Hu, teaches an algorithm for detecting topological symmetry. Similarly, Fan, like Hu and Shelley, is concerned with the detection of equivalent atoms." (Response, page 16). Thus, taken together, the cited references do not teach each limitation of claim 1. Accordingly, claim 1 is not obvious in view of Hu, Shelley, or Fan, further in view of the Helson thesis. Claims 9, 28, and 35 have comparable limitations to those of claim 1. Accordingly, these claims, as well as the claims that depend from them, are not obvious in view of the cited references.

CONCLUSION

In view of the foregoing remarks, Applicants believe that the pending application is in condition for allowance, which action is respectfully requested. If the Examiner believes that a telephone conference would expedite prosecution, the Examiner is asked to contact the undersigned.

The time for responding to this action has been extended to July 25, 2008 by the accompanying Petition for a Three Month Extension of Time and payment of fee. The Director is hereby authorized to charge Deposit Account 08-0219 the fee of $1,050 for the three-month extension of time. Please charge any other fees that may be due, or credit any overpayments to

our Deposit Account No. 08-0219, under Order No. 0103544.00131US2 from which the undersigned is authorized to draw.

Respectfully submitted,

Dated: July 25, 2008

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